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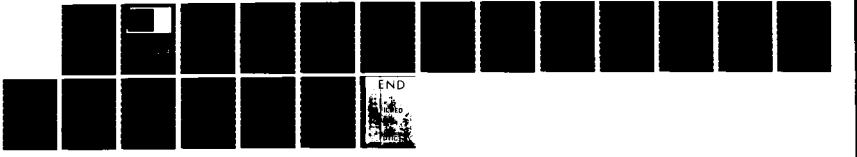

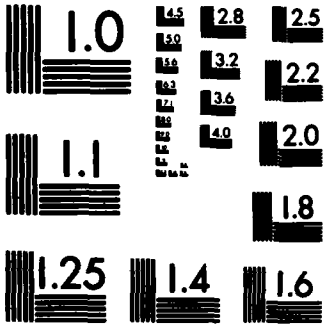

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J. L. Ericksen

Mathematics Research Center
University of Wisconsin—Madison
610 Walnut Street
Madison, Wisconsin 53705

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ABSTRACT

Commonly, hypotheses introduced by Cauchy or Born are used to relate macroscopic deformation to atomic motions, in molecular theories of elasticity. Our purpose is to discuss the applicability of these to crystal-crystal phase transformations and the ambiguities which are involved in estimating the deformation from observations of lattice vectors.

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*Department of Aerospace Engineering and Mechanics and School of Mathematics, University of Minnesota, Minneapolis, MN 55455

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THE CAUCHY AND BORN HYPOTHESES FOR CRYSTALS

J. L. Ericksen*

1. INTRODUCTION.

Commonly, molecular theories of crystal elasticity lean upon hypotheses introduced by Cauchy [1-3] or Born [4] to relate changes in atomic positions to macroscopic deformation. Both men pictured the atoms as mass points. Briefly and roughly, Cauchy assumed that atomic motion and gross motion are the same, where both are defined. Later, it was appreciated, in particular by Born, that, in a solid which appears to be at rest, atoms still undergo vibratory (thermal) motions about equilibrium positions. Since such things as x-ray observations average out such fluctuations, they can appear to be in good agreement with Cauchy's hypothesis. By these standards, Cauchy's hypothesis might or might not describe deformations encountered in transitions observed in crystals. For purposes of discussion, I will ignore such fluctuations. Born pointed out that, in some cases, Cauchy's hypothesis is in trouble for a different reason, being inconsistent with certain conditions of equilibrium. As an alternative, he proposed that lattice vectors deform as would material line elements, subject to the macroscopic deformation, the aforementioned equilibrium conditions being used to fix the finer details of atomic arrangement. In particular cases, this leads to deformations consistent with Cauchy's hypothesis. Commonly, studies requiring such an hypothesis use one of the two.

In trying to apply, or to decide whether either hypothesis is applicable to deformations involved in phase transformations, one encounters ambiguities, complicating the matter. My primary purpose is to elaborate this.

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2. THE HYPOTHESES.

A classical definition of crystals pictures configurations of atoms, filling all of space. To be crystal configurations, these must have a periodic structure, described by a translation group, generated by three (constant) linearly independent vectors, a_1, a_2 and a_3. The idea is that any point must be carried to a physically indistinguishable point by all translations of the form

$$n^K a_K \ , \tag{2.1}$$

where we use the summation convention, and the n^K represent any set of integers. What is sometimes left unsaid, but to be understood, is that this group is maximal; we don't skip over any indistinguishable points. For example, we commonly picture amorphous solids as homogeneous, meaning that we have such a translation group for any choice of a_K, but a crystallographer would not include them. With this understanding, the a_K are called lattice vectors. Less than maximal groups are sometimes encountered in practice, as will become clear. Different sets of lattice vectors are equivalent, in the sense that they generate the same translation group. For two sets a_K and $\bar{a}_K$ to be equivalent, it is necessary and sufficient that they be related by an equation of the form

$$\bar{a}_K = m^L_K a_L \ , \tag{2.2}$$

where the m^L_K are any integers such that

$$\det.\|m^L_K\| = \pm 1 \ , \tag{2.3}$$

describing the equivalence as a representation of an infinite discrete group G, which plays an important role in the classical theory of crystallographic groups. A monatomic crystal may or may not occur as a so-called simple or Bravais lattice, doing so provided application of the translation group to one atom gives the positions of all.

Of course, we observe bodies which are not infinite, but, finite. If a body, or some macroscopic part of it, can reasonably be identified with a restriction of the ideal infinite crystal, the part passes as a crystal. In the process, one exercises some judgment about defects occurring in real crystals. One crystal might, after a phase transition, exist as a number of crystals somehow joined together. It can be hard to know just what part of the original configuration corresponds to a given part of the final, let

alone decide exactly what deformation it experienced. Clearly, deciding which of an identical set of atoms goes where involves some guesswork. As is discussed by Nishiyama [5, Ch. 6], for example, metallurgists have had some limited success unravelling such puzzles. Among the ideas used is Cauchy's. Actually, some bodies of interest consist of parts which are not true crystals, but strongly resemble them. For, say, common carbon steels, the iron atoms can form a good simple lattice, but carbon atoms are distributed rather randomly. For present purposes, such things might well be regarded as crystals.

In dealing with the ideal infinite configurations, it seems fairly natural to assume, as Born did, that deformations taking one to another are homogeneous, the deformation gradient $\mathbf{F}$ being constant. Here we assume that some such configuration is taken as a reference, with some definite choice of reference lattice vectors $\mathbf{A}_K$. The Born hypothesis then reads

$$\mathbf{a}_K = \mathbf{F}\mathbf{A}_K \ , \tag{2.4}$$

the $\mathbf{a}_K$ being a possible set of lattice vectors in the deformed crystal. Given $\mathbf{A}_K$ and $\mathbf{F}$, we clearly get just one of the infinitely possible choices of lattice vectors for the deformed crystal, it being a matter of chance whether these are the same lattice vectors which an x-ray crystallographer would select. Clearly, (2.4) describes a linear transformation so, in particular, for any element of G, we have

$$m^L{}_K \mathbf{a}_K = \mathbf{F}(m^L{}_K \mathbf{A}_K) \ , \tag{2.5}$$

from which one can see that the validity of the Born hypothesis does not really depend upon a special choice of the reference lattice vectors. For a simple lattice deforming to a simple lattice, (2.4) rather suggests, as many would assume, that the atom originally at $n^K\mathbf{A}_K$ moves to $n^K\mathbf{a}_K$, ignoring a trivial translation. If so, it is consistent with Cauchy's hypothesis. Conversely, it is not hard to show that an homogeneous deformation taking a simple lattice to another will, if it is consistent with Cauchy's hypothesis, satisfy (2.4), for some choice of lattice vectors. Similar agreement occurs in some other cases, not in others. Of course, in itself, (2.4) says nothing about the fate of individual atoms, only about the periodicity of sets which they form. Thus, some assumptions are added, in making such comparison.

It seems pretty clear that (2.4) fails to apply to some of the kinds of continuous or second-order transformations considered by Landau [6], who did not discuss $\mathbf{F}$ or the equivalent, avoiding the need for accepting any particular hypothesis about it. Briefly and roughly, atomic positions are assumed to shift in a continuous way with pressure and temperature, but there can be, say, a sudden doubling in length of a lattice vector. More precisely, no matter how we select lattice vectors, at least one experiences a sizeable discontinuity. To see that this is possible one need only appreciate that the precise periodicity can be changed considerably, by infinitesimal shifts in positions of some atoms. Here, (2.4) would require $\mathbf{F}$ to suffer an unbelievably large discontinuity. Cauchy's hypothesis seems much more reasonable, on the face of it. To accept it, one must argue that the macroscopic $\mathbf{F}$ can vary somewhat over distances of the order of a few atomic spacings, which induces some queasiness.

The latter type of difficulty becomes still more severe in so-called shuffle transformations. Here, lattice vectors, chosen in an obvious way, remain fixed. So does $\mathbf{F}$, as observations are interpreted. This is consistent with (2.4), so Born's hypothesis can be considered to apply. However, some atoms in a unit cell undergo finite displacements, to symmetry-related positions. Certainly, it does not seem very reasonable to consider that Cauchy's hypothesis is applicable to such cases.

While these hypothesis have their faults, they deserve serious consideration, so we should clearly understand just what they imply. In part, this is complicated by ambiguities inherent in either. We now focus on some associated with the Born hypothesis, there being rather similar kinds associated with Cauchy's.

3. LATTICE-INVARIANT DEFORMATIONS.

Even when the Born rule applies, with $\mathbf{F}$ constant, the previous discussion makes clear that measurements of lattice vectors alone do not suffice to determine $\mathbf{F}$ uniquely. Said differently, infinitely many homogeneous deformations, which I call lattice-invariant deformations, take the ideal infinite crystal onto itself, in a manner consistent with the Born rule.

Consider any crystal configuration as a reference, and take any possible set of lattice vectors $\mathbf{a}_K$ as a reference set. From (2.2) and (2.4), we see that $\mathbf{F}$ can reasonably be considered to describe a lattice-invariant deformation provided there is some element of the group G such that

$$\mathbf{F}\mathbf{a}_K = m_K^L \mathbf{a}_L \ . \tag{3.1}$$

Mathematically, such $\mathbf{F}$ merely form a different representation of G or, if you like, a conjugate group. Introducing the dual basis $\mathbf{a}^K$, the so-called reciprocal lattice vectors, such that

$$\mathbf{a}_K \cdot \mathbf{a}^L = \delta_K^L \ , \qquad \mathbf{a}_K \otimes \mathbf{a}^K = \mathbf{1} \ , \tag{3.2}$$

we can solve (3.1) for $\mathbf{F}$, obtaining

$$\mathbf{F} = m_K^L \mathbf{a}_L \otimes \mathbf{a}^K \ . \tag{3.3}$$

Commonly, $\mathbf{F}$ is understood to be orientation preserving, so

$$\det \mathbf{F} > 0 \ , \tag{3.4}$$

Assuming this, we are restricted to the subgroup of G whose elements have positive determinant and, using (2.3), we find that (3.3) implies that

$$\det \mathbf{F} = 1 \ . \tag{3.5}$$

Since such deformations take the infinite crystal to an indistinguishable configuration, superposing a lattice-invariant deformation on any deformation should leave invariant such things as elastic strain energy functions or associated Cauchy stress tensors, at least as I and some others see it. Molecular theory of elasticity seems to support this view. When Nishiyama [5, p. 339] argues that the Bain deformation is most reasonable because it has the smallest strain energy, he seems to espouse a contrary view. Given this and other similar statements in the metallurgical literature, it seems unfair to claim that the

assertion is commonly accepted. Parry [7-8] and Pitteri [9] present analyses helpful in constructing constitutive equations exhibiting the aforementioned invariance. Of course, Born's hypothesis might hold in cases where elasticity theory fails to apply. Rivlin [10] discusses some cases which might be regarded as illustrating the possibility. Then, the usual ideas of strain energy and stress require some modification, to fit some different kind of theory.

One can push the motion a bit further, to consider the possibility that $\mathbf{F}$ is not constant, but piecewise constant. This seems reasonable, as long as the diameter of a set on which $\mathbf{F}$ is constant is reasonably large, compared to atomic spacing. Roughly, this is measured by the lengths of lattice vectors, selected to be a short as possible. In a rather natural way, this leads to a notion of lattice-invariant shears, similar to that used by metallurgists, in attempts to describe rather complex deformations encountered in some martensitic transformations. The discussion by James [11] is likely to be more accessible to those trained in mathematics or continuum mechanics.

Suppose that two neighboring parts undergo homogeneous deformations relative to some homogeneous configuration, with deformation gradients $\mathbf{F}_1$ and $\mathbf{F}_2$. We can define the relative deformation gradient $\mathbf{F}$ by

$$\mathbf{F}_2 = \mathbf{F}\mathbf{F}_1 \,, \tag{3.6}$$

what would be the deformation gradient if we took as a reference the obvious homogeneous extrapolation of the first part. Picture some part of this reference as undergoing the deformation corresponding to $\mathbf{F}$, with the gradient having a finite discontinuity on a plane with unit normal initially ν, say. We assume that the displacement remains continuous. The usual kinematical conditions of compatibility then imply that

$$\mathbf{F} = \mathbf{1} + \alpha \otimes \nu \,, \tag{3.7}$$

where α is some constant vector, not the null vector. Actually, the same condition obtains if we assume that the displacement has a constant jump discontinuity, as might be associated with slip, one of the possibilities considered by metallurgists. Second, we assume that $\mathbf{F}$ is a restriction of a lattice invariant deformation. This is, if a_K are lattice vectors in the first region, we must have, for some element of G,

$$F = 1 + a \otimes \nu = m^L_K a_L \otimes a^K . \tag{3.8}$$

Here, a definite choice of a_K might be dictated to be obtained from the original reference set by applying F, using the Born rule. As an x-ray crystallographer would see it, lattice vectors then remain continuous.

In particular, (3.5) now applies, giving

$$\det F = 1 \iff a \cdot \nu = 0 . \tag{3.9}$$

Thus, F has the form commonly associated with a simple shearing deformation, making it natural to call these <u>lattice-invariant shears</u>. Some metallurgists seem to use the term to include such things as martensitic twinning, involving a discontinuity in lattice vectors which is quite apparent from x-ray observations. According to theories of elasticity, invariant in the manner indicated, it is not automatic that stresses in such twins will be the same, although one will be unstressed if the other is. Common analyses of these employ a relation which is similar to, but different from (3.8). Some special features of equilibrium under zero stress are discussed by James [11]. Similar considerations apply to cases where the Cauchy stress reduces to an hydrostatic pressure.

Particular examples can be defined by

$$Fa_1 = a_1, \quad Fa_2 = na_1 + a_2, \quad Fa_3 = a_3 , \tag{3.10}$$

where n is any integer, a_K any linearly independent vectors, considered as lattice vectors. Here, solving for F gives

$$F = 1 + na_1 \otimes a^2 . \tag{3.11}$$

Here, we have

$$\begin{aligned} a &= \pm n a_1 |a^2| , \\ \nu &= \pm a^2 / |a^2| . \end{aligned} \tag{3.12}$$

Clearly, we here take

$$|m^L_K| = \begin{Vmatrix} 1 & 0 & 0 \\ n & 1 & 0 \\ 0 & 0 & 1 \end{Vmatrix} , \tag{3.13}$$

which, being a unimodular matrix of integers, is in G. In a certain sense, all

possibilities are of this kind. Suppose we have F, a_K, and m^K_L, satisfying (3.1). We can take any other element of G, say $\bar{m}^K_L$, and define an equivalent set of lattice vectors $\bar{a}_K$ by

$$\bar{a}_K = \bar{m}^L_K a_L \ , \tag{3.14}$$

with

$$\begin{aligned} F\bar{a}_K &= \bar{m}^L_K F a_L = \bar{m}^L_K m^P_L a_P \ , \\ &= \bar{m}^L_K m^P_L (m^{-1})^Q_P \bar{a}_Q \ , \\ &= \bar{m}^L_K \bar{a}_L \ . \end{aligned} \tag{3.15}$$

Here, we have denoted in an obvious way the inverse of the group element used. Clearly, $\bar{m}^L_K$ represents an element of G, obtained from m^L_K by applying a similarity transformation, selected as an arbitrary element of G. The allegation is that, given any solution to the problem indicated, we can use such similarity transformations to reduce it to the form described by (3.10)-(3.10).

To begin to establish this, solve (3.8) for m^K_L, which gives

$$m^L_K = \delta^L_K + \alpha^L \nu_K \ , \tag{3.16}$$

where

$$\left.\begin{aligned} \nu_K &= \nu \cdot a_K \ , \\ \alpha^L &= \alpha \cdot a^L \ . \end{aligned}\right\} \tag{3.17}$$

We have, using (3.2) and (3.9),

$$\alpha^L \nu_L = \alpha \cdot a^L \ \text{@} \ a_L \nu = \alpha \cdot \nu = 0 \ . \tag{3.18}$$

Generally, α^L and ν_K won't be integers,but the m^L_K must be. For any $\lambda \neq 0$, we will have

$$\beta^L \mu_K = \alpha^L \nu_K \tag{3.19}$$

if

$$\beta^L = \lambda \alpha^L, \quad \mu_K = (1/\lambda)\nu_K \ . \tag{3.20}$$

By properly choosing λ, we can arrange that the β^L are all integers, the μ_K rational

numbers. For example, if $\nu_1 \neq 0$, take $\lambda = 1/\nu_1$. In particular, we then know that the quantities

$$\alpha^L \nu_1 = \beta^L \mu_1 = \beta^L \tag{3.21}$$

must be integers. Assuming this, if, say, $\beta^2 \neq 0$, we know that

$$\beta^2 \mu_K \tag{3.22}$$

must be integers, requiring the μ_K to be rational numbers. One can say more about them, but this will suffice. Similarity transformations of the type allowed will take

$$\alpha_K^L = \delta_K^L + \beta^L \mu_K \tag{3.23}$$

to elements of the same form, say

$$\bar{\alpha}_K^L = \delta_K^L + \bar{\beta}^L \bar{\mu}_K \tag{3.24}$$

where the $\bar{\beta}^L$ are linear functions of the β^K with integer coefficients, $\bar{\mu}_K$ similarly related to μ_K. Thus the former will again be integers, the latter rationals. Also, (3.18) implies that

$$\beta^K \mu_K = \bar{\beta}^K \bar{\mu}_K = 0 \ . \tag{3.25}$$

Starting with this information, it is straight forward to use an elementary theorem in number theory to construct algorithms for calculating the similarity transformations needed to effect the indicated reduction, for the various possible cases.

CASE 1: Two of the β^K vanish.

By a possible transformation, renumbering lattice vectors, we can assume that

$$\beta^1 \neq 0, \ \beta^2 = \beta^3 = 0 \ , \tag{3.26}$$

whence follows from (3.25) that

$$\mu_1 = 0 \ . \tag{3.27}$$

If either μ_2 or μ_3 vanishes again renumber to get $\mu_3 = 0$. We then know that

$$\beta^1 \mu_2 = n \ ,$$

where n is some integer. This gives us (3.13). If $\mu_2 \mu_3 \neq 0$, we know that, for some integers n_2 and n_3, we have

$$\begin{aligned} \beta^1 \mu_2 &= n_2 \ , \\ \beta^1 \mu_3 &= n_3 \ , \end{aligned} \tag{3.28}$$

If n is the greatest common divisor of these integers, so that the integers

$$p_2 = n_2/n, \quad p_3 = n_3/n \tag{3.29}$$

are relatively prime, it is an elementary theorem in number theory that there exist integers q and r such that

$$p_2 q - p_3 r = 1 . \tag{3.30}$$

A possible transformation, described in terms of reciprocal lattice vectors, is then given by

$$\left.\begin{aligned} \bar{a}^1 &= a^1 , \\ \bar{a}^2 &= p_2 a^2 + p_3 a^3 , \\ \bar{a}^3 &= r a^2 + q a^3 , \end{aligned}\right\}$$

which implies that $\bar{a}_1 = a_1$. Thus,

$$\left.\begin{aligned} F &= 1 + \beta^1 a_1 \circledcirc (\mu_2 a^2 + \mu_3 a^3) , \\ &= 1 + n\bar{a}_1 \circledcirc (p_2 a^2 + p_3 a^3) , \\ &= 1 + n\bar{a}_1 \circledcirc \bar{a}^2 , \end{aligned}\right\} \tag{3.31}$$

giving us the reduction to (3.11).

CASE 2: One of the β^K vanishes.

As before, renumber to get $\beta^3 = 0$. With m as the greatest common divisor of β^1 and β^2, write

$$\beta^1 = mp^1, \quad \beta^2 = mp^2 , \tag{3.32}$$

now letting q and r be integers such that

$$p^1 q - p^2 r = 1 . \tag{3.33}$$

With the allowable change of lattice vectors given by

$$\left.\begin{aligned} \bar{a}_1 &= p^1 a_1 + p^2 a_2 , \\ \bar{a}_2 &= r a_1 + q a_2 , \\ \bar{a}_3 &= a_3 , \end{aligned}\right\} \tag{3.34}$$

we have

$$\begin{aligned} \beta^K a_K &= m(p^1 a_1 + p^2 a_2) = m\bar{a}_1 \\ &= \bar{\beta}^K \bar{a}_K , \end{aligned} \tag{3.35}$$

or $\bar{\beta}^2 = \bar{\beta}^3 = 0$. Applying to this the analysis described in CASE I then gives the desired reduction.

CASE 3: The β^K are all non-zero.

Here write

$$\beta^2 = m p^2, \quad \beta^3 = m p^3 , \tag{3.36}$$

with p^2 and p^3 relatively prime, now choosing integers q and r so that

$$p^2 q - p^3 r = 1 . \tag{3.37}$$

The change of lattice vectors given by

$$\left.\begin{aligned} \bar{a}_1 &= a_1 , \\ \bar{a}_2 &= p^2 a_2 + p^3 a_3 , \\ \bar{a}_3 &= r a_2 + q a_3 , \end{aligned}\right\} \tag{3.38}$$

then gives

$$\begin{aligned} \beta^K a_K &= \beta^1 a_1 + m(p^2 a_2 + p^3 a_3) \\ &= \beta^1 \bar{a}_1 + m \bar{a}_2 = \bar{\beta}^K \bar{a}_K , \end{aligned} \tag{3.39}$$

reducing this to CASE 2.

To sum up, if β^K and μ_L are, respectively, integers and rational numbers, (3.23) defines an element of G provided the numbers also satisfy (3.25) and the condition that the products $\beta^K \mu_L$ be integers. With a_K taken as a possible selection of lattice vectors, F, given by (3.8) defines one of the possible lattice-invariant shears. By using the above algorithms, we can always find lattice vectors reducing any possible F to the form (3.11). Said differently, ν must be parallel to a possible reciprocal lattice vector, α to one of the corresponding perpendicular lattice vectors, its magnitude being limited by (3.12).

Rather obviously, such discontinuities give rise to discontinuities in lattice vectors which agree with the Born rule, although the x-ray crystallographer would perceive lattice vectors as constant throughout. Perhaps it only reflects my lack of ingenuity, but I find it difficult to seriously consider anything more general than piecewise homogeneous deformations, as a real ambiguity involved in relating the Born hypothesis to measurements of lattice vectors. Of course, the metallurgist uses other clues, pondering how finite crystals are seen to be shaped, fit together, etc. It is not entirely easy to sort out all of the mathematical and mechanical ideas which might be involved in such considerations.

4. PRACTICE.

It is not so hard for the uninitiated to be misled by common descriptions of configurations. In a certain temperature range, a monatomic crystal might adopt a configuration sometimes described as a face-centered cubic. At other temperatures, it might occur in the form described as body-centered cubic. Different phases of iron are of these forms, for example. The words suggest picturing an homogeneous deformation of one cube to another. Apart from a rather inconsequential translation and rotation, this could only be a uniform dilation, all directions being stretched the same, a conformal mapping. Experience contradicts this, and it is inconsistent with the Cauchy and Born hypotheses.

For the face-centered cubic, the words suggest a translation group generated by three orthogonal vectors of equal length; forming edges of a cube, say b_1, b_2 and b_3. Application of this translation group to one atom, located at the origin, would generate a simple lattice, a simple cubic configuration. To get the face centered variety, we add identical atoms at three places, say

$$\tfrac{1}{2}(b_1 + b_2),\ \tfrac{1}{2}(b_2 + b_3),\ \tfrac{1}{2}(b_3 + b_1)\ , \tag{4.1}$$

applying the same translation group to these, to locate positions of remainder. Or, equivalently, we place atoms at positions whose components, relative to this basis, are either integers or half-integers.

In discussing deformations likely to occur in transitions of the kind mentioned, metallurgists sometimes picture the configuration in a different way, as a body-centered tetragonal. Here one introduces as translation vectors c_K, given by

$$\left.\begin{aligned} c_1 &= \tfrac{1}{2}(b_1 - b_2)\ , \\ c_2 &= \tfrac{1}{2}(b_1 + b_2)\ , \\ c_3 &= b_3\ , \end{aligned}\right\} \tag{4.2}$$

still orthogonal, with c_1 and c_2, but not c_3 of equal length, describing edges to the tetragon. With the factors of $\tfrac{1}{2}$ occurring, the two sets are not related by G. From this alone, it follows that not both can be lattice vectors. Application of the second group to an atom at $\tfrac{1}{2}(b_1 + b_2)$ generates most atomic positions. To get the rest, similarly

translate an atom whose position vector, relative to this point, is

$$\tfrac{1}{2}(b_1 + b_2 + b_3) \ . \tag{4.3}$$

Another way of describing the same configuration is to introduce translation vectors

$$\left.\begin{aligned} a_1 &= \tfrac{1}{2}(b_1 - b_2) = c_1 \ , \\ a_2 &= \tfrac{1}{2}(b_1 + b_2) = c_2 \ , \\ a_3 &= \tfrac{1}{2}(b_1 + b_3) = \tfrac{1}{2}(c_1 + c_2 + c_3) \ , \end{aligned}\right\} \tag{4.4}$$

Applied to one atom, this generates the whole set, describing it as a simple lattice, these a_K being one of the possible sets of lattice vectors. With the factors of $\frac{1}{2}$ running in (4.4), neither b_K nor c_K can be lattice vectors. In the jargon used by Ericksen [12], they are sub-lattice vectors. Generally sub-lattice vectors b_K are related to lattice vectors by equations of the form

$$b_K = n_K^L a_L \ , \tag{4.5}$$

where the n_K^L are integers such that

$$\det\|n_K^L\| \neq 0, \ 1, \ -1 \ , \tag{4.6}$$

so the inverse transformation exists, with coefficients which are rational numbers, not all integers. In at least some cases where the Born hypothesis fails, a modification can reasonably be applied, with lattice vectors replaced by suitably selected sub-lattice vectors. Of course, this makes the hypothesis still more ambiguous.

For the body-centered cubic, we also introduce three orthogonal vectors d_K of equal length, like the previous b_K. From an atom at the origin, this again generates a simple cubic lattice. Add an atom at

$$\tfrac{1}{2}(d_1 + d_2 + d_3) \ , \tag{4.7}$$

and similarly translate it to complete the configuration. Again, this is a simple lattice, with one set of lattice vectors $\hat{a}_K$ being given by

$$\left.\begin{aligned} \hat{a}_1 &= d_1 \ , \\ \hat{a}_2 &= d_2 \ , \\ \hat{a}_3 &= \tfrac{1}{2}(d_1 + d_2 + d_3) \ , \end{aligned}\right\} \tag{4.8}$$

and, again, the d_K are sub-lattice vectors, but not lattice vectors. The descriptions as face-or body-centered cubes have some merit, making rather obvious the crystallographic

point groups appropriate for these. By a routine calculation, one can get this from the simple lattice description. The body-centered tetragonal description suggests a different point group, and it is less routine to correctly calculate the point group, using it, but it makes it easier to picture some relevant deformations. According to either the Cauchy or the Born hypothesis, which here agree, a possible homogeneous deformation taking the face-centered cubic to the body-centered cubic configuration is defined in terms of lattice vectors described above by, as the deformation with gradient F such that

$$\hat{a}_K = Fa_K \,. \tag{4.9}$$

Of course, one can superpose lattice-invariant deformations, as described earlier, including use of lattice-invariant shears. On theoretical grounds, I see no easy way of deciding that one of these is more likely to be observed than another, although one expects them to be separated by energy barriers. With (4.9), elementary calculations indicate that one can picture the deformation as that taking the tetragon with edges c_K to the cube with edges d_K, a deformation which is clearly different from the uniform dilatation mentioned at the beginning of this section. In the metallurgical literature, this is called the Bain distortion or Bain deformation. Some discussions of this such as that of Nishiyama [5, p. 339] mention experimental confirmation that this is the deformation which occurs in at least some cases. Following this is a discussion of martensitic transformations which involve much more complex patterns of deformation, with quite different crystal configurations contacting each other. Certainly, it would be nice to have better tools, to resolve such puzzles.

In this discussion, I glossed a point. Conceivably, the uniform dilatation and the deformation given by (4.9) could both be consistent with the Born hypothesis. It is not very hard to show that they can't, but I won't take space to elaborate this.

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Commonly, hypotheses introduced by Cauchy or Born are used to relate macroscopic deformation to atomic motions, in molecular theories of elasticity. Our purpose is to discuss the applicability of these to crystal-crystal phase transformations and the ambiguities which are involved in estimating the deformation from observations of lattice vectors.

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